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Computation of the Rate of Solidification of an Ingot Taking into Account the Temperature Dependence of the Thermophysical Parameters of the Metal

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In computing the rate of advance of the crystallization front during solidification of a metal ingot, one usually assumes that the thermal conductivity λ and the heat capacity c of a solid metal are independent of the temperature. The average values of the thermophysical parameters of the substances $\bar{\lambda}$ and \bar{c} in the given temperature range are used in the computation. As the range is extended, the actual values of λ and c may, at certain temperatures T , differ considerably from $\bar{\lambda}$ and \bar{c} . The error thus introduced into the result remains undetermined, and therefore the validity of using $\bar{\lambda}$ and \bar{c} instead of the actual thermophysical parameters of the metal is doubtful. To solve the problem of the possibility of computing the solidification rate of the metal with sufficient accuracy while limiting ourselves to $\bar{\lambda}$ and \bar{c} , we must have a more accurate method enabling us to allow for the temperature dependence of λ and c .

In this paper we try to develop such a method, which could be used for various dependences of λ and c on T . For concreteness we assume

$$\lambda = \lambda_0 + \mu T, \quad c = c_0 + \omega T. \quad (1)$$

The relation between λ , c , and T corresponding to equations (1) applies to many metals and alloys in a wide temperature range. For most metals, we have $\mu < 0$, $\omega > 0$.

We shall assume that there is no superheating of the melt and that the temperature of the metal depends only on the distance from the surface of the ingot and on the time t (reference 2). The equation describing the variation of the temperature in the solidified crust of the metal has the form

$$\frac{\partial}{\partial x} \left[(\lambda_0 + \mu T) \frac{\partial T}{\partial x} \right] = \gamma (c_0 + \omega T) \frac{\partial T}{\partial t}, \quad (2)$$

where γ is the density of the metal;

$$T(x, 0) = T_{cr} \quad \text{for } x > 0, \quad (3)$$

where T_{cr} is the crystallization temperature of the metal.

If a constant temperature is preserved at the surface of the ingot during crystallization, we have, for $t > 0$,

$$T(0, t) = T_0, \quad (4)$$

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where T_0 is the temperature of the surface of the ingot.

On the crystallization front $x = y(t)$, where $y(t)$ is the coordinate of the crystallization front, increasing with time,

$$T[y(t), t] = T_{cr}. \quad (5)$$

From the condition of heat balance at the melt-liquid [sic] phase boundary, we obtain

$$\frac{\partial y}{\partial t} = \frac{\lambda_0 + \mu T_{cr}}{Q\gamma} \left(\frac{\partial T}{\partial x} \right)_{x=y(t)}, \quad (6)$$

where Q is the heat of crystallization per gram.

We introduce the quantities:

$$\begin{aligned} \bar{\lambda} &= \lambda_0 + \mu \frac{T_{cr} + T_0}{2}; & \bar{c} &= c_0 + \omega \frac{T_{cr} + T_0}{2}; \\ \Theta &= \frac{2}{T_{cr} - T_0} \left(T - \frac{T_0 + T_{cr}}{2} \right); \\ \bar{a} &= \frac{\lambda}{\gamma c}; & \alpha_1 &= \frac{\mu (T_{cr} - T_0)}{2\bar{\lambda}}; & \alpha_2 &= \frac{\omega (T_{cr} - T_0)}{2\bar{c}}; & q &= \frac{2Q}{\bar{c} (T_{cr} - T_0)}. \end{aligned} \quad (7)$$

The conditions of our problem can be written as

$$\begin{aligned} \frac{\partial}{\partial x} \left[(1 + \alpha_1 \Theta) \frac{\partial \Theta}{\partial x} \right] &= \frac{1}{\bar{a}} (1 + \alpha_2 \Theta) \frac{\partial \Theta}{\partial t}; & \Theta(0, t) &= -1; \\ \Theta[y(t), t] &= 1; & \frac{dy}{dt} &= \frac{\bar{a}}{q} (1 + \alpha_1) \left(\frac{\partial \Theta}{\partial x} \right)_{x=y(t)}. \end{aligned} \quad (8)$$

We shall seek

$$\Theta(x, t) \equiv \Theta(u); \quad u = \frac{x}{\sqrt{2at}}; \quad y(t) = \beta \sqrt{2at}, \quad (9)$$

where β is an unknown constant.

Hence

$$\frac{d}{du} \left[(1 + \alpha_1 \Theta) \frac{d\Theta}{du} \right] + u (1 + \alpha_2 \Theta) \frac{d\Theta}{du} = 0; \quad (10)$$

$$\Theta(0) = -1; \quad (11)$$

$$\Theta(\beta) = 1; \quad (12)$$

$$\beta = \frac{1 + \alpha_1}{q} \left(\frac{d\Theta}{du} \right)_{u=\beta}. \quad (13)$$

The case $\alpha_1 = \alpha_2 = 0$ corresponds to taking the average values for λ and c in the entire temperature range from T_{cr} to T_0 . Then

$$\frac{d^2\Theta}{du^2} + u \frac{d\Theta}{du} = 0; \quad (14)$$

$$\Theta(0) = -1; \quad (15)$$

$$\Theta(\bar{\beta}) = 1; \quad (16)$$

$$\left(\frac{d\Theta}{du} \right)_{u=\bar{\beta}} = \bar{\beta} q; \quad (17)$$

here $\bar{\beta}$ is the value of β computed from the average values of λ and c .

The solution of Eq. (14) with due regard for the conditions in (15) and (16) has the form

$$\Theta = \frac{\operatorname{erf}(u/V\sqrt{2})}{\operatorname{erf}(\bar{\beta}/V\sqrt{2})} - 1; \quad \operatorname{erf} z = \frac{2}{V\pi} \int_0^z e^{-t^2} dt. \quad (18)$$

Condition (17) results in the transcendental equation determining the value of $\bar{\beta}$:

$$\operatorname{erf}\left(\frac{\bar{\beta}}{V\sqrt{2}}\right) e^{-(\bar{\beta})^2/2} \bar{\beta} q = \frac{2\sqrt{2}}{V\pi}. \quad (19)$$

Since

$$\operatorname{erf}\left(\frac{\bar{\beta}}{V\sqrt{2}}\right) = \frac{2}{V\pi} e^{-(\bar{\beta})^2/2} \sum_{k=0}^{\infty} \frac{2^k \left(\frac{\bar{\beta}}{V\sqrt{2}}\right)^{2k+1}}{1 \cdot 3 \cdot 5 \cdot 7 \cdots (2k+1)}, \quad (20)$$

it follows from (19) that

$$\frac{2}{q} = (\bar{\beta})^2 + \frac{1}{1 \cdot 3} (\bar{\beta})^4 + \frac{1}{1 \cdot 3 \cdot 5} (\bar{\beta})^6 + \frac{1}{1 \cdot 3 \cdot 5 \cdot 7} (\bar{\beta})^8 + \dots \quad (21)$$

The solution of Eq. (10) can be written in the form of the series

$$\Theta(u) = \sum_{n=0}^{\infty} \left(\frac{d^n \Theta}{du^n} \right)_{u=\beta} \frac{(u-\beta)^n}{n!}. \quad (22)$$

It can be seen from conditions (12) and (13) that

$$\Theta(\beta) = 1; \quad \left(\frac{d\Theta}{du} \right)_{u=\beta} = \frac{q\beta}{1 + \alpha_1}. \quad (23)$$

By successive differentiation of Eq. (10), we find the derivatives of the function $\Theta(u)$ of higher order for $u = \beta$:

$$\left(\frac{d^2 \Theta}{du^2} \right)_{u=\beta} = -\beta^2 \left[\frac{1 + \alpha_2}{(1 + \alpha_1)^2} q + \frac{\alpha_1}{(1 + \alpha_1)^2} q^2 \right]; \quad (24)$$

$$\left(\frac{d^3 \Theta}{du^3} \right)_{u=\beta} = -\beta \frac{1 + \alpha_2}{(1 + \alpha_1)^3} q + \beta^2 \left[\frac{(1 + \alpha_2)^2}{(1 + \alpha_1)^3} q + \frac{4\alpha_1 + 3\alpha_1\alpha_2 - \alpha_2}{(1 + \alpha_1)^4} q^2 + \frac{3\alpha_1^3}{(1 + \alpha_1)^5} q^3 \right]; \quad (25)$$

$$\begin{aligned} \left(\frac{d^4 \Theta}{du^4} \right)_{u=\beta} = & \beta^2 \left[\frac{3(1 + \alpha_2)^2}{(1 + \alpha_1)^5} q + \frac{6\alpha_1 + 4\alpha_1\alpha_2 - 2\alpha_2}{(1 + \alpha_1)^6} q^2 \right] - \beta^4 \left[\frac{(1 + \alpha_2)^3}{(1 + \alpha_1)^7} q + \right. \\ & \left. + \frac{(1 + \alpha_2)(11\alpha_1 + 7\alpha_1\alpha_2 - 4\alpha_2)}{(1 + \alpha_1)^8} q^2 + \frac{\alpha_1(25\alpha_1 + 18\alpha_1\alpha_2 - 7\alpha_2)}{(1 + \alpha_1)^9} q^3 + \frac{15\alpha_1^3}{(1 + \alpha_1)^{10}} q^4 \right] \end{aligned} \quad (26)$$

etc.

According to condition (11)

$$-1 = \sum_{n=0}^{\infty} (-1)^n \left(\frac{d^n \Theta}{du^n} \right)_{u=\beta} \frac{\beta^n}{n!}. \quad (27)$$

Substituting equations (24), (25), (26), etc., into (27), we obtain after certain transformations a series of even powers of the required constant β :

$$\begin{aligned} \frac{2}{q} (1 + \alpha_1) = & \beta^2 + \beta^4 \left[\frac{1 + \alpha_2}{3(1 + \alpha_1)} + \frac{\alpha_1}{2(1 + \alpha_1)^2} q \right] + \beta^6 \left[\frac{(1 + \alpha_2)^2}{15(1 + \alpha_1)^3} + \right. \\ & \left. + \frac{5\alpha_1 + 4\alpha_1\alpha_2 - \alpha_2}{12(1 + \alpha_1)^4} q + \frac{\alpha_1^2}{2(1 + \alpha_1)^5} q^2 \right] + \beta^8 \left[\frac{(1 + \alpha_2)^3}{105(1 + \alpha_1)^5} + \frac{(1 + \alpha_2)(31\alpha_1 + 22\alpha_1\alpha_2 - 9\alpha_2)}{180(1 + \alpha_1)^6} q + \right. \\ & \left. + \frac{\alpha_1(19\alpha_1 + 15\alpha_1\alpha_2 - 4\alpha_2)}{30(1 + \alpha_1)^7} q^2 + \frac{5\alpha_1^3}{8(1 + \alpha_1)^8} q^3 \right] + \dots \end{aligned} \quad (28)$$

It is easy to see that for $\alpha_1 = \alpha_2 = 0$ the series (28) is transformed into the series (21).

When the values α_1 and α_2 are given concretely, the convergence of the series (28) is studied by the usual methods.

Expression (28) is a transcendental equation from which it is possible to determine the value of β graphically or by the method of inversion of the power series. When β is known it is easy to calculate the rate of advance of the crystallization front during the solidification of the metal ingot:

$$v = \frac{dy}{dt} = \frac{\beta \sqrt{\frac{a}{2t}}}{V} . \quad (29)$$

In the case of a more complex dependence of λ and c on T , the scheme of the solution of the problem remains unchanged, except that the computation formulas will be different.

There may be cases when the computation can be made according to (21) with great accuracy and the value of β is practically the same as $\bar{\beta}$.

Let us calculate the crystallization rate of an aluminum ingot. In this case we have $Q = 95.5 \text{ cal/gm}$, $T_{cr} = 659^\circ \text{C}$, $\gamma = 2.7 \text{ gm/cm}^3$. The dependence of λ and c on T for aluminum has been reported. Analytically, the dependence of λ and c on T in a wide temperature range can be described by the formulas

$$\lambda \approx (0.5 - 0.00025T^\circ \text{C}) \frac{\text{cal}}{\text{cm} \times \text{sec} \times \text{deg}}; c = (0.2096 + 0.0001T^\circ \text{C}) \frac{\text{cal}}{\text{gm} \times \text{deg}} .$$

If we assume that $T_0 = 100^\circ \text{C}$, we have $\alpha_1 = -0.1725$; $\alpha_2 = 0.1129$; and $q = 1.3803$. From the series (28), we obtain $\beta = 1.011$. For $\alpha_1 = \alpha_2 = 0$, the computation gives $\bar{\beta} = 0.989$.

In the case under study $\beta/\bar{\beta} = 1.023$; i.e., the error in determining β caused by the temperature dependence of the thermophysical parameters of aluminum is somewhat larger than 2 percent of the computed quantity. Thus, in calculating the solidification of the aluminum ingot, we can assume with sufficient accuracy that $\beta = \bar{\beta}$.

There are possible cases in the crystallization of metals (particularly metals having a high melting point) when the difference between β and $\bar{\beta}$ is much more substantial than in the above example.

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